ALEXANDER

GASH

The Synthesis of Monolithic Transition and Main Group Metal-Oxide Aerogels from Inorganic Salt Precursors

Alexander E. Gash
Chemistry and Materials Science Directorate

We have applied a novel synthetic approach to prepare a variety of transition and main group metal-oxide aerogels via the sol-gel route. This approach is direct, inexpensive, versatile, and has been shown to produce monolithic mesoporous materials (pore diameters from 3-23 nm) with high surface areas (200-600 m^2/g). Both pH and nuclear magnetic resonance (NMR) studies suggest that a proton scavenger allows the ionic metal species to undergo hydrolysis and condensation to form a metal-oxide framework. Preliminary studies suggests that metal-oxide gels should be attainable using most metal salt precursors, provided a suitable nucleophilic anion is also present in solution. Characterization of the solid materials using X-ray powder diffraction, X-ray absorption spectroscopy, scanning and transmission electron microscopy, surface area (BET) and pore size distribution will also be discussed.

SOPHIA

HAYES

Characterization of GaAs Semiconductors and Development of Optically Polarized Solid-State NMR Methods

Sophia Hayes

Abstract

Both bulk and low-dimensional semiconductor structures of GaAs such as nanoclusters have been characterized by various techniques, including x-ray diffraction, Auger electron spectroscopy, x-ray photoelectron spectroscopy, photoluminescence, and solid-state optically polarized NMR.

We have developed optically polarized NMR (OPNMR) equipment to study these materials in order to gain a better understanding of their structure and electronic properties. Optical pumping of semiconductor materials has been utilized to achieve NMR sensitivity enhancements in III-V and II-VI semiconductors. We will present some results for optical pumping using irradiation above the bandgap, incrementing laser polarization settings, temperature dependence, and laser power.

We are also investigating how chemical passivation of these semiconductor surfaces affects both the photoluminescence and solid-state NMR spectra.

MARY

MC BRIDE

Determining the Structure of Biomaterials Interfaces Using Synchrotron-based X-ray Diffraction

M. McBride, C.A. Orme, A. Noy, J.J. DeYoreo

Our ability to control either the production of natural biomaterials or the reaction of the body to synthetic biomaterials must begin with an understanding of the physics and chemistry of deposition and dissolution at solid-liquid interfaces in biological systems. Developing this understanding requires experimental tools for probing surface and near-surface atomic structure in fluids. We have examined the feasibility of using synchrotron-based surface X-ray diffraction (SXRD) to determine the surface structure of biominerals in solution and the adsorbed layer of acidic amino acids that are believed to play a central role in the control of biomineral form and function.

Our results show that the binding of aspartic acid (ASP) to calcite results in features observed in biomineralized systems, including the stabilization of non-equilibrium facets. We find that chiral amino acids break the calcite crystal symmetry and cause the emergence of chiral structures. From bulk and surface spectroscopic analysis, we find that ASP is not present within the bulk of the crystals, nor is it adsorbed in any appreciable amount on the {104} face. Crystallographic modeling shows that binding to the {110} and {1-10} faces is preferred over binding to the {104} face and that L- and D-ASP have different binding energies. Based on these results we propose that the modification of calcite growth by acidic amino acids results from changes to the calcite surface and step free energies in response to stereo-specific binding to the {hk0} step risers. These results establish an important step towards understanding how the more complex peptides and proteins found in living organisms act to control carbonate mineralization.

MOON

RHEE

Simulation of Early Stage Deformation of Molybdenum Using 3D Dislocation Dynamics

Moon Rhee
Chemistry and Materials Science Directorate
MSTD, Lawrence Livermore National Laboratory
Livermore, CA 94550

Collaborators: Vasily Bulatov, David Lassila, Luke Hsuing, Tomas Diaz de la Rubia

Abstract

Early stages of plastic deformation and the underlying dislocation behavior in Mo are examined using a recently developed dislocation dynamics code (*micro3d*), where dislocation curves of arbitrary shapes are discretized into sets of straight segments of mixed dislocations. The interactions among the segments, including line tension and self interactions, are treated explicitly. For longer-range interactions, the space is divided into a regular cellular array and the elastic fields of the remote cells are approximated by a mulipolar expansion. Initial dislocation arrangements were generated to mimic realistic TEM dislocation microstructures in the annealed Mo single crystals. The simulated deformation response indicates the onset of plastic yield and the development of characteristic cross-grid patterns dominated by the long screw dislocations. Multiplication occurs naturally at the pinning points formed by non-coplanar superjogs moving towards each other along the screw dislocations. We present a detailed analysis of the developing dislocation microstructures revealing their contribution to the observed yield behavior.

SHARON SHIELDS

Methods and Principles in Energy Filtering Transmission Electron Microscopy (EFTEM)

Jürgen M. Plitzko
Chemistry and Materials Science Directorate, University of California, Lawrence Livermore National Laboratory P.O. Box 808, Livermore, CA 94550

During the past 10 years the field of energy filtering transmission electron microscopy (TEM) has grown rapidly. It started to show its use to solve material science problems in the last couple of years. The story of the energy filter began with its invention in the sixties, followed by the theoretical development of the omega filter in the seventies until the first energy filtered TEM's of the later type were commercially available in the late eighties.
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KEVIN VANDERSALL

Combined Electromagnetic Particle Velocity and Manganin Pressure Gauge Technique for Non steady Wave Analysis

Kevin S. Vandersall
Energetic Materials Program Element
Supervisor: Jerry Forbes

Use of electromagnetic particle velocity (EMV) gauges and manganin piezoresistive stress gauges are common experimental techniques used to make in-situ measurements in shock wave experiments. Using the conservation jump equations along with initial parameters and in-situ measurements allows the conditions during the experiment to be understood if a steady wave is assumed. However, if a steady wave is not present (such as commonly seen in energetic materials) then a non steady wave analysis must be employed involving a more complex set of differential equations in place of the conservation jump equations. This analysis then requires that two parameters (such as particle velocity and pressure) be measured simultaneously to solve these equations.Because of this interest, some preliminary experiments have been performed to investigate measuring particle velocity and pressure at the same time using combined EMV and manganin gauges. Combining these techniques offers complexity due to the nature of electrical and electromagnetic interaction. This talk will provide background on both the non steady wave analysis and the experimental techniques utilized as well as describe and discuss the preliminary results and offer insightinto future planned experiments.

ELIZABETH WHEELER

Methods and Principles in Energy Filtering Transmission Electron Microscopy (EFTEM)

Jürgen M. Plitzko
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JENNIFER YOUNG

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DARIO

ARENA

Photoemission Studies of the α and δ Phases of Plutonium at the Advanced Light Source

D.A. Arena1, J.G. Tobin1, J. Terry2, R. Schulze2, J. Lashley2, J. D. Farr2, T. Zocco2, D. Shuh3, E. Rotenberg3

1Lawrence Livermore National Lab
2Los Alamos National Lab
3Lawrence Berkeley National Lab

Metallic plutonium has one of the most complex and intriguing structural phase diagrams on the periodic table. Of particular importance are the low symmetry, high density α (monoclinic) phase and the higher symmetry, lower density δ (fcc) phase. We examined the α and δ allotropic phases of Pu using high resolution soft X-ray photoemission (XPS) and resonant photoemission spectroscopy (ResPES) conducted at the Spectromicroscopy Facility at the Advanced Light Source of Lawrence Berkeley National Lab and have identified several pronounced differences in the photoemission spectra between the two phases. The core level XPS spectra of the 4f7/2 spectral line from both α– and δ-Pu samples exhibit a sharp peak metallic peak which is indicative of a core hole that is readily screened by de-localized electrons. However, the screening is enhanced in the α-Pu spectrum, which suggests a larger degree of de-localization in α-Pu than in δ-Pu. A similar picture emerges from the valence band ResPES measurements. In those data, the resonant enhancement of the valence band signal was more pronounced in δ-Pu than in α-Pu. Such an increased resonant enhancement is consistent with a greater degree of localization in δ-Pu.

The felicity afforded by the use of a synchrotron as the excitation source also allows us to more accurately determine the cleanliness of our Pu samples. Spectra acquired at photon energies corresponding to laboratory XPS sources show little oxidation of the samples. Spectra acquired at lower photon energies, which enhances the sensitivity to the O 1s level, indicate that non-negligible amounts of oxygen are present in samples that were thought to be clean. As a result, we are currently constructing an improved spectrometer and vacuum system which will minimize the interval between sample cleaning and data acquisition. Such a system shall allow us to systematically examine the development of oxidation on Pu and other highly reactive samples. The system is also designed to heat and cool the sample *in-situ* and thus allow us to follow the changes in the electronic structure of metallic Pu as it undergoes the transformation from the α-phase through the δ-phase.

NERINE

CHEREPY

Direct Conversion of Carbon Anode Fuels into Electricity

Nerine Cherepy, Roger Krueger and John F. Cooper
Chemistry and Materials Science Directorate
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The direct electrochemical conversion of carbon to electricity involves discharge of suspensions of reactive carbon against an oxygen (air) cathode. The free energy and the enthalpy of the oxidation reaction are nearly identical, allowing theoretical efficiencies ($\Delta G/\Delta H$) approaching 100% and consequently low thermal loads. The activities of the elemental carbon and of the carbon dioxide product are invariant. This stabilizes cell EMF and allows high fuel utilization. Finally, the energy cost for pyrolysis of hydrocarbons (4-10% of fuel value) is very low compared with that of the steam reforming or water gas reactions typically used to convert methane into hydrogen for use in fuel cells.

We report new data on the electrochemical behavior of carbon anode slurries, finely-divided carbons in a molten carbonate electrolyte. The cell separator is a wetted porous ceramic material, with an anode current collector on one side, contacting the carbon slurry, and a cathode current collector on the other side. The cathode reaction gas is a mixture of air and carbon dioxide, while the anode atmosphere is a combination of inert gas and CO2 (or CO2 only).

Cathode:	$O2 + 2CO_2 + 4e-$	$= 2CO_3^{2-}$
Anode:	$C + 2CO_3^{2-}$	$= 3CO_2 + 4e-$
Total Reaction:	$C + O_2$	$= CO_2$

At typical operating temperatures, 700-850 °C, open circuit potentials of 1.0-1.2 V are measured, and at 0.8 V cell potential, current densities from 5 to 100 mA/cm2 are reported. The broad range of measured discharge rates (current densities) correlates to the reactivity of different carbon fuels. We are presently exploring the relationship between micro- and nanostructure of carbon fuels and their electrochemical reactivity. Measured peak powers of 80-100 mW/cm2 lie within the practical range for power sources such as fuel cells and primary batteries.

Applications include baseload utility and carbon/oxygen primary batteries.

ACKNOWLEDGEMENTS
This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

MICHAEL HOSCHSTRASSER

Fermi Surfaces and Magnetic Behavior of Thin FeNi Alloy Films

M. Hochstrasser and J.G. Tobin
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N.A.R. Gilman, and R.F. Willis, *Department of Physics, The Pennsylvania State University, PA 16802*
F.O. Schumann, *Physik Departement, Freie Universität Berlin, 14195 Berlin, Germany*
E. Rotenberg, *Advanced Light Source, Lawrence Berkeley National Laboratory, CA 94720*

We report angle-resolved and spin-resolved photoemission measurements of changes in the electronic structure with changing composition of pseudomorphic films of FeNi magnetic alloys grown epitaxially on Cu(100). With x-ray magnetic linear dichroism angle-dependent (XMLDAD) 3p core-level photoemission the evolution of the elemental magnetic moments was monitored. In addition changes occurring in the spin-polarized valence bands were observed with spin-polarized photoemission, together with changes in the k-distribution of states at the Fermi energy.
A <110> projection of the Fermi surface shows a delocalized “dogbone” feature due to sp-states and more localized “hotspots” corresponding to the emergence of minority spin d-states. Hybridization between the sp- and d-states occurs a these locations on the dogbone indicative to a strong nesting of wavevectors of excitations spanning the Fermi surface. The sp-dogbone states spin polarize with increasing average magnetic moment.
Both elemental moments, observed in XMLDAD, grow with increasing Fe concentration up to a maximum at the Fe concentration of 55%, that on the Fe increasing at a faster rate than the Ni moment. Beyond this point, the Fe moment shows a rapid decline to a “low-spin” value, of the order of that of the Ni moment, which tracks the behavior of the Fe moment but to a smaller degree. Spin-resolved valence band photoemission measurements show first an increase in the exchange splitting of the 3d-states, followed by a decline, essentially tracking the core-level dichroism.
The magnetic instability observed above the invar concentration (Fe>65%) is charac-terized further by a diffuseness in the spectral distribution and an increased lifetime broadening of mainly minority-spin states, indicative of magnetic non-collinear disorder.

ALISON KUBOTA

Development of Empirical Potentials for Molecular Dynamics Simulations and Their Application

Alison Kubota, William J. Pitz and Charles K. Westbrook, LLNL
Maria Caturla, Vasily Bulatov, Tom Lenosky and Tomas Diaz de la Rubia, LLNL
Pierre-A. Glaude, CNRS, Nancy, France
Joseph W. Bozzelli, New Jersey Institute of Technology, NJ, USA
Richard Wise and Alois Gutmann, IBM and Siemens DRAM Development Alliance, Hopewell Junction, New York, USA

In this poster, we present ongoing work on several projects spanning the field of atomistic computational chemistry in different areas, addressing issues relevant to current industrial and programmatic needs. We demonstrate the capabilities to both develop and implement the necessary tools.

In microelectronics processing applications, molecular dynamics is increasingly being used to investigate the role of energetic particles in the radiation damage of electronic material surfaces. One particular problem of great interest to the microelectronics industry is in the area of photolithography. Patterned photoresists are used in reactive plasmas to assist in etching sub-micron scale features on electronic material surfaces. Erosion resistance, or the ability for the photoresist to resist etching, is a feature which needs to be improved for 193 and 157nm applications. We present work demonstrating the capability to quickly develop Brenner-type interatomic multi-element reactive bond order potentials. Such potentials are required in order to simulate large systems consisting of many thousands of atoms, over hundreds of picoseconds, and when bond-breaking and bond-forming processes are to be modelled. Furthermore, such potentials improves the predictive capabilities to test arbitrary polymers and plasma-chemistry, towards the development of new erosion-resistant materials.

In the development of Brenner-type potentials for photoresists, the thermodynamic properties for many oxygenated species must be calculated. This properties are also needed in the area of chemical kinetic modeling of oxygenated fuels which is an area of interest in our Computational Chemistry group. Addition of oxygenated hydrocarbons to conventional fuels has been shown to reduce soot emissions in diesel engines and CO emissions in spark-ignition engines. The elimination of MTBE as an oxygenated additive to gasoline has created an interest in alternative oxygenated additives to achieve legislated goals in pollutant emission reduction. Interest in oxygenated fuels has created a need for the thermodynamic parameters of these fuels and for their intermediate and radical breakdown products. We present accurate thermochemical data on large oxygenated hydrocarbon species (R(OH)n and R(OCH3)n using the CBS-Q composite ab initio and density functional method. The enthalpy of formation is calculated with the inclusion of conformational mixing, and and isodesmic reactions, with group balance when possible. We find that for many polymethoxy alkane species, that the enthalpy of formation (H298) is reproduced to within 1.1 kcal/mol. We also observe C-O bond stabilization with increasing methoxy and hydroxyl substitution, likely attributed to the anomeric effect.

Currently, one of the most urgent priorities of the National Ignition Facility is the mitigation of crack propagation and damage growth in the laser optics. Much experimental characterization has been done in the attempt to understand the mechanism of both the damage initiation and growth. In this project, we have developed the capability to simulate crack growth under extreme conditions of pressure, temperature and loading conditions, using molecular dynamics, in the attempt to elucidate the growth process at the atomic scale. In particular, we have implemented an reactive bond-order charge-transfer modified Born-Mayer-Huggins potential to a massively-parallel MD code.

CARoLA

LAUE

Exploring the Elements of Our Periodic Table

Carola A Laue, Heavy Element Group—Glen T. Seaborg Institute for Transactinum Science, Analytical and Nuclear Chemistry Division, CMS—LLNL

Since the beginning of the so-called alchemy, the exploration of basic chemical properties of the elements has always fascinated the chemists. As we add more and more elements to our periodic table, exploring basic chemical properties becomes more challenging, complex and exciting.
Three new elements (114, 116, and 118) were added to the Periodic Table within the last year. Studying these elements seems to be far out of reach, but not impossible. Over the last decades, studies on element 104 through 107 have shown, that low production rates (e.g. one atom per day), short half-lives (as small as 10 to 20 sec), and strong interference due to transfer and other unwanted products can not halter the chemists enthusiasm.
Several new (potentially useful in the future) approaches to improve one or the other factors limiting the studies of the chemical properties will be indicated as for instance: the use of radioactive beams to produce more neutron rich and hence more stable transactinides; the use of an ion-trap to explore spectral properties; or even the potential use of nano-technology, which could provide a more efficient way to perform the chemical studies.
Ongoing first studies of the -homologe group (Si-Ge-Sn-Pb) of element 114 will be highlighted. Simple adsorption behavior of the homologe elements on a lead-specific extraction resin is expected to yield information on the gradual transition of the oxidation state from +4 to +2 within the group. Performing the same study on element 114 would answer the question of its oxidation state.

ALEKSANDR NOY

Scanning Probe Microscopy of Molecular Interactions

Aleksandr Noy

Progress in he emerging field of nanotechnology depends on our ability to observe, manipulate and create nanostructures at the interfaces. Scanning probe microscopy (SPM) plays a central role in these efforts due to its unique combination of near-atomic spatial resolution, and ability to work in ambient conditions. We will discuss our ongoing effort in developing SPM capabilities with the ultimate goal of assembling a versatile nanotechnology tool kit.

Size, geometry and mechanical properties of carbon nanotubes makes them ideal candidates for creating the ultimate probe microscopy tips. We will discuss the advantages of such probes, the approaches for fabricating them and some of their application to high-resolution imaging of biological objects. We will also show our initial efforts in nanoscale surface patterning using SPM nanolithography. Finally, we will discuss our strategies for integrating scanning probe microscopy with single molecule optical detection for developing ways to identify and map single molecules and their interactions on surfaces.

JURGEN PLITZCO

Methods and Principles in Energy Filtering Transmission Electron Microscopy (EFTEM)

Jürgen M. Plitzko
Chemistry and Materials Science Directorate, University of California, Lawrence Livermore National Laboratory P.O. Box 808, Livermore, CA 94550

During the past 10 years the field of energy filtering transmission electron microscopy (TEM) has grown rapidly. It started to show its use to solve material science problems in the last couple of years. The story of the energy filter began with its invention in the sixties, followed by the theoretical development of the omega filter in the seventies until the first energy filtered TEM's of the later type were commercially available in the late eighties.

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MARK SUTTON

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ANA VILLACAMPA

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LI8A

WICKHAM

Dislocation dynamics simulations at small and large scale, using the PARANOID code.

LISA WICKHAM

Large scale dislocation-dynamics simulations can use elastic theory to describe long-range interactions between dislocations, but they also need an efficient way to treat close dislocation encounters. We have used the high spatial resolution of the PARANOID dislocation dynamics code to study such encounters and choose a rule for predicting when dislocations will come together in bound junction states, which contribute to work hardening. We have verified that this line-tension based rule is sufficient in a wide variety of situations, which include external stress and dislocation curvature. In addition, we have found that dislocations can come together in a crossed configuration which is moderately bound but does not zip up into a junction.In ongoing work, we are using these rules in larger-scale simulations of various dislocation configurations that are motivated by TEM observations of dislocations in bcc metals. These include screw dislocations with jog densities designed to match statistics from TEM observations of annealed molybdenum, and dislocation tangles which contain junctions, since such structures are observed to develop under work hardening. We are also continuing to test and improve the capabilities of the code, which include good scalability and the recent addition of periodic boundary conditions, designed to prevent any artificial loss of dislocations through a computational cell boundary.